

Journal of

Computational Physics

VOLUME 52, 1983



ACADEMIC PRESS

Subsidiary of Harcourt Brace Jovanovich, Publishers

New York London

Iris San Diego San Francisco São Paulo Sydney Tokyo Toronto

Copyright © 1983 by Academic Press, Inc.

All Rights Reserved

No part of this publication may be reproduced or transmitted in any form or by any means, electronic or mechanical, including photocopy, recording, or any information storage and retrieval system, without permission in writing from the copyright owner.

The appearance of the code at the bottom of the first page of an article in this journal indicates the copyright owner's consent that copies of the article may be made for personal or internal use, or for the personal or internal use of specific clients. This consent is given on the condition, however, that the copier pay the stated per copy fee through the Copyright Clearance Center, Inc. (21 Congress Street, Salem, Massachusetts 01970), for copying beyond that permitted by Sections 107 or 108 of the U.S. Copyright Law. This consent does not extend to other kinds of copying, such as copying for general distribution, for advertising or promotional purposes, for creating new collective works, or for resale. Copy fees for pre-1983 articles are as shown on the article title pages; if no fee code appears on the title page, the copy fee is the same as for current articles.

0021-9991/83 \$3.00

Printed by the St. Catherine Press, Ltd., Bruges, Belgium

CONTENTS OF VOLUME 52

NUMBER 1, OCTOBER 1983

VIEW ARTICLE

| | |
|--|-----|
| CLIVE TEMPERTON. Self-Sorting Mixed-Radix Fast Fourier Transforms | 1 |
| ANS C. ANDERSEN. Rattle: A "Velocity" Version of the Shake Algorithm for Molecular Dynamics Calculations | 24 |
| KOSLOFF AND R. KOSLOFF. A Fourier Method Solution for the Time Dependent Schrödinger Equation as a Tool in Molecular Dynamics | 35 |
| M I.-P. SHIH, GENE E. SMITH, GEORGE S. SPRINGER, AND Y. RIMON. Boundary Conditions for the Solution of Compressible Navier-Stokes Equations by an Implicit Factored Method | 54 |
| OMAS KAIJSER. A Simple Inversion Method for Determining Aerosol Size Distributions | 80 |
| KANNAN AND W. PROSKUROWSKI. A Numerical Method for the Nonlinear Neumann Problem | 105 |
| CUPINI, A. DE MATTEIS, AND R. SIMONINI. Monte Carlo Simulation of the Charge-Transfer Reaction in a Plasma | 122 |
| ENJI INOUE. Grid Generation for Cascades Using Conformal Mapping | 130 |
| JAMES G. BERRYMAN. Computing Variational Bounds for Flow through Random Aggregates of Spheres | 142 |
| EL DIERCKX. An Algorithm for Experimental Data Deconvolution Using Spline Functions | 163 |
| BETANCOURT, F. HERRNEGGER, P. MERKEL, J. NÜHRENBURG, R. GRUBER, AND F. TROYON. Comparison of MHD Stability Results Obtained with the BETA 3D and HERA 2D Codes | 187 |

NOTES

| | |
|---|-----|
| CLIVE TEMPERTON. A Note on Prime Factor FFT Algorithms | 198 |
| M. G. BROWN AND J. W. DUNGEY. Economising Plasma Simulation by Total Neglect of the Displacement Current | 205 |
| GIOIETTA KUO-PETRAVIC. Numerical Treatment of the Axial Singularity in a Flux Coordinate System for Particle Simulation | 209 |
| SØREN TOXVAERD. Energy Conservation in Molecular Dynamics | 214 |
| ST OF FORTHCOMING ARTICLES | 217 |

NUMBER 2, NOVEMBER 1983

| | |
|--|-----|
| OTSUKA, M. NAGAMI, AND T. MATSUDA. Birth: A Neutral Beam Deposition for Non-Circular Tokamak Plasmas | 219 |
| I. MARCHUK AND V. I. KUZIN. On the Combination of Finite Element and Splitting-Up Methods in the Solution of Parabolic Equations | 237 |

| | |
|---|-----|
| J. M. SANZ-SERNA AND V. S. MANORANJAN. A Method for the Integration in Time of Certain Partial Differential Equations | 273 |
| M. G. G. FOREMAN. An Analysis of the "Wave Equation" Model for Finite Element Tidal Computations | 290 |
| I. M. NAVON. A Numerov-Galerkin Technique Applied to a Finite-Element Shallow-Water Equations Model with Enforced Conservation of Integral Invariants and Selective Lumping | 313 |
| CLIVE TEMPERTON. Fast Mixed-Radix Real Fourier Transforms | 340 |
| NORMAN J. ZABUSKY AND EDWARD A. OVERMAN II. Regularization of Contour Dynamical Algorithms. I. Tangential Regularization | 351 |
| J. J. MONAGHAN AND R. A. GINGOLD. Shock Simulation by the Particle Method SPH | 374 |
| A. NISHIGUCHI AND T. YABE. Second-Order Fluid Particle Scheme | 390 |
| DIMITRI HATZIAVRAMIDIS AND HWAR-CHING KU. Pseudospectral Solutions of Laminar Heat Transfer Problems in Pipelines | 414 |
| LIST OF FORTHCOMING ARTICLES | 425 |

NUMBER 3, DECEMBER 1983

| | |
|--|-----|
| A. R. GARLICK. The Use of Distorting Grids and Flux Splitting to Model Axisymmetric Adiabatic Explosions | 427 |
| S. C. R. DENNIS AND L. QUARTEPPELLE. Direct Solution of the Vorticity-Stream Function Ordinary Differential Equations by a Chebyshev Approximation | 448 |
| J. C. T. WANG. On the Numerical Methods for the Singular Parabolic Equations in Fluid Dynamics | 464 |
| D. C. BARNES, T. KAMIMURA, J.-N. LEBOEUF, AND T. TAJIMA. Implicit Particle Simulation of Magnetized Plasmas | 480 |
| S. H. JOHNSON AND A. C. HINDMARSH. Numerical Dynamic Simulation of Solid-Fluid Reactions in Isothermal Porous Spheres | 503 |
| R. D. MOSER, P. MOIN, AND A. LEONARD. A Spectral Numerical Method for the Navier-Stokes Equations with Applications to Taylor-Couette Flow | 524 |
| I. DILBER, J. M. WALSH, AND J. DENAVIT. Convergence of Stochastic Orbit Computations | 543 |
| J. B. BELL AND G. R. SHUBIN. An Adaptive Grid Finite Difference Method for Conservation Laws | 569 |
| JOHN D. RAMSHAW. A Method for Enforcing the Solenoidal Condition on Magnetic Field in Numerical Calculations | 593 |

NOTE

| | |
|---|----|
| H. YAMAMOTO. An Efficient Algorithm for Calculating Thrust in High Multiplicity Reactions | 59 |
|---|----|

| | |
|--|----|
| LIST OF FORTHCOMING ARTICLES | 60 |
| AUTHOR INDEX FOR VOLUME 52 | 60 |

Journal of Computational Physics

INFORMATION FOR AUTHORS

The purpose of the *Journal of Computational Physics* is to publish articles concerning techniques developed in the solution of data handling problems and mathematical equations, both arising in the description of physical phenomena.

Manuscripts should be submitted to: *Journal of Computational Physics*, Lawrence Livermore National Laboratory, University of California, P. O. Box 5509, L-561, Livermore, California, 94550.

Original papers only will be considered. Manuscripts are accepted for review with the understanding that the same work has not been and will not be published nor is presently submitted elsewhere, and that persons listed as authors have given their approval for the submission of the paper; further, that any person cited as a source of personal communications has approved such citation. Written authorization may be required at the Editor's discretion. Articles and any other material published in the *Journal of Computational Physics* represent the opinions of the author(s) and should not be construed to reflect the opinions of the Editor(s) and the Publisher.

Authors submitting a manuscript do so on the understanding that if it is accepted for publication, copyright in the article, including the right to reproduce the article in all forms and media, shall be assigned exclusively to the Publisher. The Publisher will not refuse any reasonable request by the author for permission to reproduce any of his or her contributions to the journal.

Form of Manuscript. Manuscripts should be typewritten with wide margins on high quality 8.5×11 inch paper, using double spacing throughout. The original and two copies should be submitted; however, in order to expedite handling of manuscripts, the original and four copies would be desirable. Manuscripts should include figures and tables.

Each page of the manuscript should be numbered. The first should contain the article title, author and author names and complete affiliation(s). At the bottom of this page, the number of manuscript pages, figures, and tables should be noted. The second page should contain a proposed running head of less than thirty-five characters. It should also contain the name and complete mailing address of the person to whom proofs are to be sent.

With the exceptions noted below, authors should be guided by the *Style Manual*, 1978, of the American Institute of Physics.

Subject Classification. As of January 1981 authors are required to classify their own manuscripts using the 1980 *Mathematics Subject Classification*, reprinted from the 1978 *Mathematical Reviews*, pp. S27-S34, with the additional classifications listed in the January 1, 1981 issue. Authors are requested to choose at least two categories, one in numerical analysis category, 65, and one other, preferably a physical classification, from the categories beyond 65. Page one should contain at least two subject classification index numbers.

Abstract. Page 3 should contain a short abstract.

List of Symbols. It is of vital importance that the author submit a complete list of symbols. The symbols used should be identified for the typesetter **phonetically**. This list will not appear in print, but is essential to avoid costly corrections in proof.

Tables. Number tables consecutively with Roman numerals. Extensive tables will be reproduced as line drawings, and should be typed carefully in the **exact** format desired. Authors will be charged for new engravings necessitated by changes in proof. Use superscript lower-case italic letters (*a*, *b*, *c*) for table footnotes, which should be typed immediately below the table. Type tables at least double-spaced, including titles and footnotes. Do not underline table titles; reserve underlining for text that is to be italicized.

Equations. Equations should be typewritten whenever possible, and the number placed in parentheses at the right margin. Reference to equations should use the form "Eq. (3)" or simply "(3)". Superscripts and subscripts should be typed or handwritten clearly above and below the line, respectively. Use the exponent $^{1/2}$ whenever possible.

References. References should be cited in the text by a number in square brackets. Literature cited should appear on a separate page at the end of the article, and should be styled and punctuated according to the following examples:

1. J. G. DEE, *Ann. Phys. (N.Y.)* **61** (1969), 880.
[Underline only names of journals.]
2. R. P. SHUTT, "Bubble and Spark Chambers," Vol. 2, p. 50, Academic Press, New York/London, 1967.
3. W. B. THOMPSON, Kinetic Theory of Plasma, in "Advanced Plasma Theory" (M. N. Rosenbluth, Ed.), Chap. 1, Academic Press, New York, 1964.

For unpublished lectures or symposia, include title of the paper, name of the sponsoring society in full, and date. For journal names, follow the style of *Chemical Abstracts Service Source Index*, 1980. Abbreviation of AEC Laboratory Report names should follow the style of *Nuclear Science Abstracts*.

Footnotes. Footnotes in the text should be avoided if at all possible. If they must be used, identify by superscript numbers and type together on a separate page, double spaced.

Figures. All illustrations are to be considered as figures. Number each graph or drawing in sequence with Arabic numerals. Supply a descriptive legend for each figure. Type legends double-spaced consecutively on a separate page. The **original** figures are required. Copies are **unacceptable**.

Plan figures to fit the proportion of the printed page. Use a professional lettering set on the original so that the letters and numbers are large enough and "open" enough to take a reduction of 50 to 60% without filling in with ink. Do not include background grids; however, on paper with blue lines the grid can be eliminated in the process of photoreproduction. Identify each figure in a margin with the name of the journal, author's name, and figure numbers; avoid marking the backs of figures.

Proofs. Galley proofs will be sent to the author with a reprint order form. Authors will be charged for alterations in excess of 10% of the cost of composition.

Reprints. Fifty reprints without covers will be provided free of charge. Additional reprints may be purchased.

Notes

Short notes regarding the availability of interesting and useful new programs or tabular material will be considered for publication. Letters to the Editor commenting on articles already published in this Journal will also be considered. Neither notes nor letters should have an abstract.